

Velocity, temperature and normal force dependence on friction: An analytical and molecular dynamic study

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In this work we propose an extension to the analytical one-dimensional model proposed by E. Gnecco (Phys. Rev. Lett. 84:1172) to describe friction. Our model includes normal forces and the dependence with the angular direction of movement in which the object is dragged over a surface. The presence of the normal force in the model allow us to define judiciously the friction coefficient, instead of introducing it as an *a posteriori* concept. We compare the analytical results with molecular dynamics simulations. The simulated model corresponds to a tip sliding over a surface. The tip is simulated as a single particle interacting with a surface through a Lennard-Jones (6 – 12) potential. The surface is considered as consisting of a regular BCC(001) arrangement of particles interacting with each other through a Lennard-Jones (6 – 12) potential. We investigate the system under several conditions of velocity, temperature and normal forces. Our analytical results are in very good agreement with those obtained by the simulations and with experimental results from E. Riedo (Phys. Rev. Lett. 91:084502) and Eui-Sung Yoon (Wear 259:1424-1431) as well.

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I. INTRODUCTION

Understanding the origin of tribological phenomena is a fascinating and challenging enterprise. The classical point of view of the frictional phenomena, can be synthesized in the three laws of friction, valid in the macroscopic scale [1, 2]:

1. Friction is independent of the apparent area of contact,
2. Friction is proportional to the applied load. The ratio between the friction force and the applied load is named the coefficient of friction ($\mu = f_L/f_N$) and it is larger for static friction than for kinetic friction,
3. Kinetic friction is independent of the relative sliding velocity.

Since new tools, such as the atomic force microscopy (AFM), have made possible to examine the friction phenomenon in great detail these laws have been questioned in systems with dimensions approaching the nanometer scale. At the same time, the development of ultra fast computers have allowed to test new theories on the nano-scale friction world. Although tribology is an old science, and in spite of the efforts and progress made by scientists and engineers in the last years, tribology is still far from being a well-understood subject. In fact, it is incredible that even knowing several properties as surface energy, elastic properties and loss properties, a friction coefficient cannot be found by using an *a priori* calculation. Although in the macroscopic scale the friction force, f_L , is independent of the relative velocity, in the nanometric scale some authors [3, 4, 5, 6] observed that the mean value of the friction force presents a logarithmic velocity dependence. Another important result was the conclusion that friction force is proportional to the effective contact area down to the nanometer scale [7]. An analytical one-dimensional model known as Tomlinson model [1] was able to explain several features of the nanoscopic friction. Using the Tomlinson model in the limit of

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low velocities Gneco et al [3] showed that the friction force has a logarithmic dependence with the velocity. Using the same ideas, but in the limit of higher velocities, Sang et al. [8] obtained that the friction force is proportional to $|\ln(v)|^{2/3}$, where v is the relative velocity. Using a first principle model Persson [9] was able to show that in the limit of small contact areas the result of Sang is recovered while in the limit of large contact areas the Gneco result fitted better. The aim in this work is to develop a model from first principle by extending the one-dimensional model proposed by Sang et al. [8] to three-dimensions. Based in our approach we obtain a friction coefficient which can be calculated knowing simple parameters of the model (As bound energies and the positions of the minima between atoms.). Such parameters can be obtained by using ab-initio calculations or measured experimentally by using FFM (Friction force microscopy) [3, 5, 10, 11] or DFS (Dynamic force microscopy) [12]. We study the sliding frictional process by using two approaches:

- Developing an analytic model that considers the potential energy between a atom in the tip and the surface atoms described by the model presented by W. A. Steele [13] as a sum of pair-wise (6 – 12) LJ potentials. The analytic treatment extends the one dimensional model proposed by Riedo et al.[4] including the normal force and as a consequence, the effects of adhesion energies.
- Using MD simulations by considering that the potential energy between the tip's atom and the surface atoms is described as a sum of (6 – 12) LJ potentials (See ref. [14] and references there in.).

II. FIRST PRINCIPLE MODEL

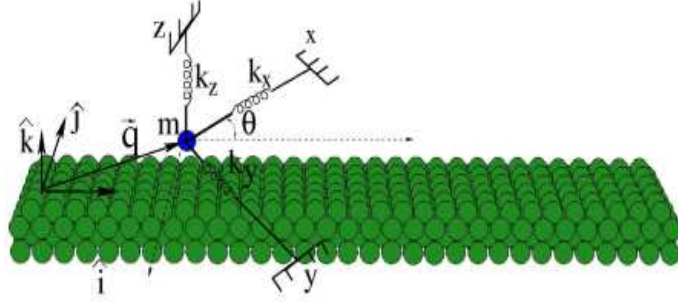


Figure 1: Perspective view of a typical initial configuration [BCC(001) geometry] for the FFM experiment.

In this section we show a general picture of the nature of the kinetic friction. Consider the sliding system shown in figure (1) in which one particle of mass m is connected through a spring to a cantilever or drive. The particle experiences a total force described by the potential [1]

$$V_{Tot} = \frac{1}{2} \left[(\vec{q} - \vec{r}) \cdot \overleftrightarrow{k} \cdot (\vec{q} - \vec{r}) \right] + V_{int}(\vec{q}), \quad (1)$$

where

$$\overleftrightarrow{k} = \begin{bmatrix} k_x & 0 & 0 \\ 0 & k_y & 0 \\ 0 & 0 & k_z \end{bmatrix} \quad (2)$$

represents the harmonic spring constant complying the cantilever with the tip, $V_{int}(\vec{q})$ is the surface-tip corrugated potential, $\vec{q} = (q_x, q_y, q_z)$ are the coordinates of the tip and $\vec{r} = (x, y, z)$ the coordinates of the support. As we are interested to study the influence of the normal force on the sliding process, let us first note that the critical state (Where we denote the drive position by $\vec{r}_c = (x_c, y_c, z_c)$ and the particle position by $\vec{q}_c = (q_{xc}, q_{yc}, q_{zc})$) is the position where the tip jumps from a stable position in the surface to the next one. To illustrate the occurrence of the critical state, we show in the figure 2 the total potential energy of the tip as a function of q_x , for two different positions of the cantilever, $x < x_c$ (full line) and $x = x_c$ (dashed line). As a matter of clarity we restrict this figure to the x direction.

From figure 2, the critical point is defined as the inflexion point of the total potential energy and mathematically it means,

$$\left. \frac{\partial V_{Tot}}{\partial \vec{q}} \right|_{\vec{q}_c, \vec{r}_c} = 0 \quad (3)$$

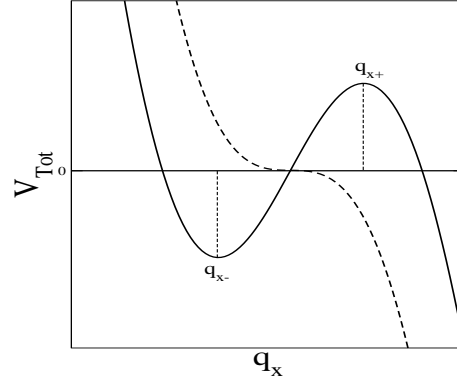


Figure 2: Schematic figure illustrating the critical state for two different positions of the cantilever, $x < x_c$ (full line) and $x = x_c$ (dashed line). The marked points define the energy barrier that prevents a jump from one stable position (q_{x-}) to another (equation 8). Figure from reference [4].

$$\left[\frac{\partial^2 V_{Tot}}{\partial q_x^2} \frac{\partial^2 V_{Tot}}{\partial q_y^2} - \left(\frac{\partial^2 V_{Tot}}{\partial q_y \partial q_x} \right)^2 \right] \bigg|_{\vec{q}_c, \vec{r}_c} = 0 \quad (4)$$

$$\frac{\partial^2 V_{Tot}}{\partial q_z^2} \bigg|_{\vec{q}_c, \vec{r}_c} > 0 \quad (5)$$

The first condition, equation (3), is always satisfied at equilibrium, it states that the total force on the particle must vanish. The second condition, equation (4), is satisfied in a transition from a stable to an instable position on the plane of the surface (critical points). It states that the determinant of the Hessian matrix in the plane vanishes. It follows from the fact that at these points, the slope of the force due to the substrate equals the slope, k_α , of the spring force. The third condition, equation (5), defines that the particle is always in contact with the surface.

We can write the total potential as $V_{Tot}(\vec{q}, \vec{r}) = V_{Tot}(\vec{q}_\parallel, \vec{r}_\parallel, q_z, z)$, where \vec{q}_\parallel and \vec{r}_\parallel are coordinates parallel to the surface and the others correspond to the normal components. We can expand the potential around the critical points, $\vec{\chi} = (\vec{q}_c, \vec{r}_c)$, as

$$\begin{aligned} V_{Tot} \approx & A(\vec{r}_\parallel, z) + (\vec{r}_\parallel - \vec{r}_{\parallel c}) \cdot \frac{\partial^2 V_{Tot}}{\partial \vec{r}_\parallel \partial \vec{q}_\parallel} \bigg|_{\vec{\chi}} \cdot (\vec{q}_\parallel - \vec{q}_{\parallel c}) \\ & + \frac{1}{3!} \frac{\partial^3 V_{Tot}}{\partial \vec{q}_\parallel^3} \bigg|_{\vec{\chi}} \cdot (\vec{q}_\parallel - \vec{q}_{\parallel c})^3 \\ & + \frac{\partial^2 V_{Tot}}{\partial z \partial q_z} \bigg|_{\vec{\chi}} (z - z_c)(q_z - q_{zc}) \\ & + 2 \frac{\partial^2 V_{Tot}}{\partial \vec{q}_\parallel \partial q_z} \bigg|_{\vec{\chi}} \cdot (\vec{q}_\parallel - \vec{q}_{\parallel c})(q_z - q_{zc}) \\ & + \frac{1}{2!} \frac{\partial^2 V_{Tot}}{\partial q_z^2} \bigg|_{\vec{\chi}} (q_z - q_{zc})^2 + \dots \end{aligned} \quad (6)$$

As a matter of clarity we write this potential in a more compact form,

$$\begin{aligned} V_{Tot} \approx & A(x, y, z) + C_1(x - x_c)(q_x - q_{xc}) \\ & + C_2(y - y_c)(q_y - q_{yc}) + C_3(z - z_c)(q_z - q_{zc}) \\ & + C_{13}(q_x - q_{xc})(q_z - q_{zc}) + (E_3/2)(q_z - q_{zc})^2 \\ & + C_{23}(q_y - q_{yc})(q_z - q_{zc}) \\ & + (E_1/6)(q_x - q_{xc})^3 + (E_2/6)(q_y - q_{yc})^3 + \dots \end{aligned} \quad (7)$$

where the constants, A , C_1 , C_2 , C_3 , C_{13} , C_{23} , E_1 , E_2 and E_3 will be explicitly written in the next section, they are immediately obtained by direct comparison with equation (6). The main goal of this model is to show that the dynamic energy barrier, ΔE , which prevents the jump of the tip from a stable equilibrium position on the surface to

the nearest neighboring one, is a function of the instantaneous lateral force, f_L , and the instantaneous normal force, f_z . The energy barrier ΔE is defined as

$$\Delta E = V_{Tot}(\vec{q}_{max}, t) - V_{Tot}(\vec{q}_{min}, t) \quad . \quad (8)$$

The quantities \vec{q}_{max} and \vec{q}_{min} correspond to the first minimum and maximum of the combined potential at time, t , it is determined by the equilibrium condition $\partial V / \partial \vec{q} = 0$ [4] (See figure 2).

Using the equilibrium condition in the equation (7) we obtain,

$$\frac{E_1}{2}(q_x - q_{xc})^2 + C_{13}(q_z - q_{zc}) + C_1(x - x_c) = 0 \quad (9)$$

$$\frac{E_2}{2}(q_y - q_{yc})^2 + C_{23}(q_z - q_{zc}) + C_2(y - y_c) = 0 \quad (10)$$

$$E_3(q_z - q_{zc}) + C_{13}(q_x - q_{xc}) + C_{23}(q_y - q_{yc}) + C_3(z - z_c) = 0 \quad (11)$$

substituting (11) in (9), (10) and holding only terms of first order in C_{13} and C_{23} , we obtain two quadratic equations in q_x , q_y to solve, whose solutions are

$$q_{x\pm} - q_{xc} = \pm \frac{1}{E_1^{1/2}} \sqrt{2C_1(x'_c - x)} \quad (12)$$

$$q_{y\pm} - q_{yc} = \pm \frac{1}{E_2^{1/2}} \sqrt{2C_2(y'_c - y)} \quad (13)$$

with

$$\begin{aligned} C_1 x'_c &= C_1 x_c - (C_{13}/E_3)C_3(z_c - z) \quad , \\ C_2 y'_c &= C_2 y_c - (C_{23}/E_3)C_3(z_c - z) \quad . \end{aligned}$$

Using the definition of ΔE , and equations from (7) to (13) we can get the energy barrier as

$$\Delta E = \frac{2^{\frac{7}{2}}}{3} \left\{ \frac{[C_1(x'_c - x)]^{3/2}}{E_1^{1/2}} + \frac{[C_2(y'_c - y)]^{3/2}}{E_2^{1/2}} \right\}. \quad (14)$$

Defining,

$$\begin{aligned} f_x(t) &= C_1 x(t) \quad ; \quad F_{xc} = C_1 x_c \quad ; \quad F'_{xc} = C_1 x'_c \quad , \\ f_y(t) &= C_2 y(t) \quad ; \quad F_{yc} = C_2 y_c \quad ; \quad F'_{yc} = C_2 y'_c \quad , \\ f_z(t) &= C_3 z(t) \quad ; \quad F_{zc} = C_3 z_c \quad , \end{aligned}$$

$$\begin{aligned} f_x(t) &= f_L(t) \cos(\theta) \quad ; \quad f_y(t) = f_L(t) \sin(\theta) \quad , \\ F_{xc} &= F_{lc} \cos(\theta) \quad ; \quad F_{yc} = F_{lc} \sin(\theta) \quad , \\ F_{lc} &= \sqrt{F_{xc}^2 + F_{yc}^2} \quad ; \quad f_L(t) = \sqrt{f_x(t)^2 + f_y(t)^2} \quad , \\ F'_{xc} &= F'_{lc} \cos(\theta) \quad ; \quad F'_{yc} = F'_{lc} \sin(\theta) \quad , \end{aligned}$$

we find an energy barrier which is similar to that found in other works [8, 9, 11],

$$\Delta E(t) = \lambda_1(\theta) \left[F'_{lc}(f_z(t)) - f_L(t) \right]^{3/2} \quad , \quad (15)$$

where,

$$\mu_{0x} = \frac{C_{13}}{E_3} \quad ; \quad \mu_{0y} = \frac{C_{23}}{E_3} \quad , \quad (16)$$

$$\lambda_1(\theta) = \frac{2^{\frac{7}{2}}}{3} \left\{ \frac{|\cos(\theta)|^{\frac{3}{2}}}{E_1^{\frac{1}{2}}} + \frac{|\sin(\theta)|^{\frac{3}{2}}}{E_2^{\frac{1}{2}}} \right\} \quad , \quad (17)$$

$$F'_{lc}(f_z(t)) = \sqrt{F_{lc}^2 + (\mu_{0x}^2 + \mu_{0y}^2)(f_z(t) - F_{zc})^2 + 2F_{lc}(\mu_{0x} \cos(\theta) + \mu_{0y} \sin(\theta))(f_z(t) - F_{zc})} \quad (18)$$

We note that ΔE presents a dependence with the instantaneous normal force, f_z , and the angle $0 \leq \theta \leq \pi$ between the direction x and the force pushing the cantilever. Now we will study the consequences of this dependence in the friction force. At zero temperature, the lateral force required to the tip jumping from a minimum to another is $f_L(t) = F'_{lc}(f_z(t))$ (i.e., the force corresponding to $\Delta E = 0$). At finite temperature, T , the occurrence of thermally activated transitions between two minima, when $\Delta E > 0$, leads to $f_L(t) < F'_{lc}(f_z(t))$ and the probability that the tip does not jump, $p(t)$, is described by the master equation [3, 4, 5, 11]:

$$\frac{\partial p(t)}{\partial t} = -\nu_0 \exp[-\beta \Delta E(t)] p(t) \quad (19)$$

where $\beta = 1/k_b T$, ν_0 is the jump frequency transition and k_b is the Boltzmann constant. Using the condition for the maximum jumping probability, $d^2 p/dt^2 = 0$, the following expression has to be satisfied:

$$\Delta E = -\frac{1}{\beta} \ln \left(-\frac{\beta}{\nu_0} \frac{d\Delta E}{dt} \right) \quad (20)$$

Then

$$\begin{aligned} \frac{df_L}{dt} &= \left[\frac{\partial f_L}{\partial f_x} \right] \left[\frac{\partial f_x}{\partial x} \right] \left[\frac{\partial x}{\partial t} \right] + \left[\frac{\partial f_L}{\partial f_y} \right] \left[\frac{\partial f_y}{\partial y} \right] \left[\frac{\partial y}{\partial t} \right] \\ &= \left[\frac{f_x}{f_L} \right] [\kappa_{eff}^x][v_x] + \left[\frac{f_y}{f_L} \right] [\kappa_{eff}^y][v_y] \\ &= (\kappa_{eff}^x \cos(\theta))^2 + \kappa_{eff}^y \sin(\theta)^2 v_l = \varphi v_l \\ \frac{dF'_{lc}}{dt} &= \left[\frac{\partial F'_{lc}}{\partial f_z} \right] \left[\frac{\partial f_z}{\partial z} \right] \left[\frac{\partial z}{\partial t} \right] = \left[\frac{\partial F'_{lc}}{\partial f_z} \right] \kappa_{eff}^z v_z \\ &= \gamma \kappa_{eff}^z v_z \\ \frac{d\Delta E}{dt} &= -\frac{3}{2} \lambda_1 [F'_{lc}(f_z) - f_L]^{1/2} \left(\frac{df_L}{dt} - \frac{dF'_{lc}}{dt} \right) \\ &= -\frac{3}{2} \lambda_1 [F'_{lc}(f_z) - f_L]^{1/2} |\varphi v_l + \gamma \kappa_{eff}^z v_z| \end{aligned} \quad (21)$$

where,

$$\begin{aligned} \varphi(\theta, f_z) &= \kappa_{eff}^x \cos(\theta)^2 + \kappa_{eff}^y \sin(\theta)^2 \\ v_x &= v_l \cos(\theta) \quad ; \quad v_y = v_l \sin(\theta) \quad ; \quad v_l = \sqrt{v_x^2 + v_y^2} \end{aligned} \quad (22)$$

$$\begin{aligned} \gamma(\theta, f_z) &= \frac{1}{F'_{lc}} \left[(\mu_{0x}^2 + \mu_{0y}^2)(f_z(t) - F_z^*) \right. \\ &\quad \left. + F_{lc}(\mu_{0x} \cos(\theta) + \mu_{0y} \sin(\theta)) \right], \end{aligned} \quad (23)$$

and κ_{eff}^α is the effective stiffness of contact [15] in the directions $\alpha = x, y, z$. It is important to stand out that $\kappa_{eff}^{x,y}$ is a function of the normal force. This dependence, will appear in a crucial way in the deduction of the theoretical coefficient of friction that we will present. The effective stiffness of contact can be experimentally determined by measuring the inclination of the “stick region”, which is the region were the tip is in a stable position before the equation (4) is satisfied in the friction force loop [16]. Thus, the effective stiffness of contact is defined as,

$$\kappa_{eff}^x = \frac{\partial f_x}{\partial x} = \left(\frac{1}{\kappa_{contact}^x} + \frac{1}{k_x} \right)^{-1}, \quad (24)$$

where $\kappa_{contact}^x$ is the stiffness of contact which is a function of the normal force [17, 18] and k_x (equation (2)), is the spring constant of the cantilever. Using equations (15), (20) and (21) we obtain the lateral force,

$$f_L = F'_{lc}(f_z) - \left\{ \frac{k_b T}{\lambda_1(\theta)} \left[\ln \left(\frac{v_0(f_z)}{|\varphi v_l - \kappa_{eff}^z \gamma v_z|} \right) - \frac{1}{2} \ln \left(1 - \frac{f_L}{F'_{lc}(f_z)} \right) \right] \right\}^{2/3} \quad (25)$$

where

$$v_0(f_z) = \frac{2\nu_0 k_b T}{3\lambda_1(\theta)(F'_{lc})^{1/2}}, \quad (26)$$

This result has a similar form to those presented by Riedo et. al [4] with three interesting physical differences: 1) the explicitly normal force dependence on $F'_{lc}(f_z)$ and $v_0(f_z)$ as indicated by experimental results [4]; 2) the angular dependence of the friction force relative to the periodic crystalline structure of the sliding surface; 3) the logarithmic normal velocity dependence of the friction force, as Jeon et. al. [19] have shown experimentally and numerically simulated using a single particle model. Note that by introducing a normal force dependence in the friction force it is natural to think of the coefficient of friction as defined by

$$\mu(t) = \frac{\partial f_L(t)}{\partial f_z(t)} = \gamma + 2 \left(\frac{k_b T}{\lambda_1} \right)^{2/3} \times \frac{\left[\frac{\partial \varphi}{\partial f_z} v_l - \kappa_{eff}^z \frac{\partial \gamma}{\partial f_z} v_z \right]}{[\varphi v_l - \kappa_{eff}^z \gamma v_z]} \frac{\left\{ \ln \left(\frac{v_0}{|\varphi v_l - \kappa_{eff}^z \gamma v_z|} \right) - \frac{1}{2} \ln \left(1 - \frac{f_L}{F'_{lc}} \right) \right\}^{2/3}}{\left\{ 1 + 3 \left[\ln \left(\frac{v_0}{|\varphi v_l - \kappa_{eff}^z \gamma v_z|} \right) - \frac{1}{2} \ln \left(1 - \frac{f_L}{F'_{lc}} \right) \right] \right\}} \quad (27)$$

where

$$\frac{\partial \varphi}{\partial f_z} = \frac{\partial \kappa_{eff}^x}{\partial f_z} \cos(\theta) + \frac{\partial \kappa_{eff}^y}{\partial f_z} \sin(\theta) \quad (28)$$

$$\frac{\partial \gamma}{\partial f_z} = \frac{F_{lc}^2 [\mu_{0x} \sin(\theta) - \mu_{0y} \cos(\theta)]^2}{(F'_{lc})^3} \quad (29)$$

Observe that this equation gives a friction coefficient that is a function of velocity, temperature, normal force and the direction that the cantilever is dragged in the surface. In the next sections we show this results for a selected potential and we compare it with MD simulations. It is important to note that if we know the potential between the surface and the tip atoms we can predict the value of the friction coefficient with no adjustable parameters.

In the next section we will use a total potential to calculate the values of the parameters defined in the model and show that the theoretical friction force agree very well with experimental results [4, 7].

III. SURFACE-TIP'S POTENTIAL AND PARAMETERS OF THE ANALYTIC MODEL

The model we developed has no adjustable parameters. Once the potential energy is given, we are able to calculate the friction force. For a well behaved surface, Steele[13] has derived a model potential which is very fair in describing the interaction with a periodic surface

$$V_{int}(\vec{q}_{||}, q_z) = V_0(q_z) + V_1(q_z) \sum_{\vec{G}} \cos(\vec{G} \cdot \vec{q}_{||}), \quad (30)$$

where $\vec{q}_{||} = (q_x, q_y)$ are the coordinates of the tip's atom parallel to the substrate and \vec{G} is the set of the six shortest reciprocal lattice vectors of the substrate. The first term in equation (30) describes the mean interaction of the atoms with the substrate, and the second term describes the periodic corrugation potential. Expressions for V_0 and V_1 were derived by Steele[13], assuming that the substrate potential $V_{int}(\vec{q})$ is a sum of LJ potentials between one film atom and all of the atoms in the substrate. The parameters of the LJ potential can nowadays be experimentally determined by DFS [20] experiments for a specific material. Other expressions for V_0 and V_1 , where described by some authors such as Persson et. al. [21], Liebsch et. al. [22] that consider these terms composed by exponentials and Tomassone et. al. [23] consider expressions that give a correct description of the interaction of a metallic surface with a noble gas atom. In this work we use the expression derived by Steele. At this point we need to define the

surface arrangement of particles which we are interested to work with. We use the regular BCC(001) surface, so that the total potential energy (Equation (1)) becomes

$$V_{Tot} = \frac{1}{2} \left[(\vec{q} - \vec{r}) \cdot \overleftrightarrow{k} \cdot (\vec{q} - \vec{r}) \right] + V_0(q_z) + 2V_1(q_z) [\cos(G_x q_x) + \cos(G_y q_y)] . \quad (31)$$

Using the conditions imposed by the equations (3) to (5) in equation (31) one obtain,

$$k_x(q_{xc} - x_c) - 2V_1(q_{zc}) \sin(G_x q_{xc}) G_x = 0 , \quad (32)$$

$$k_y(q_{yc} - y_c) - 2V_1(q_{zc}) \sin(G_y q_{yc}) G_y = 0 , \quad (33)$$

$$k_z(q_{zc} - z_c) + V_0'(q_z) + 2V_1'(q_{zc}) [\cos(G_x q_{xc}) + \cos(G_y q_{yc})] = 0 , \quad (34)$$

$$\frac{\partial^2 V_{Tot}}{\partial q_x^2} = k_x - 2V_1(q_z) \cos(G_x q_x) G_x^2 ,$$

$$\frac{\partial^2 V_{Tot}}{\partial q_y^2} = k_y - 2V_1(q_z) \cos(G_y q_y) G_y^2 ,$$

$$\frac{\partial^2 U_{Tot}}{\partial q_x \partial q_y} = 0 ,$$

$$\left[\frac{\partial^2 V_{Tot}}{\partial q_x^2} \frac{\partial^2 V_{Tot}}{\partial q_y^2} - \left(\frac{\partial^2 V_{Tot}}{\partial q_y \partial q_x} \right)^2 \right] \bigg|_{\vec{q}_c, \vec{r}_c} = 0$$

$$\begin{aligned} & [k_x - 2V_1(q_{zc}) \cos(G_x q_{xc}) G_x^2] \times \\ & [k_y - 2V_1(q_{zc}) \cos(G_y q_{yc}) G_y^2] = 0 \end{aligned} \quad (35)$$

Solving these equations we get,

$$\begin{aligned} q_{xc} &= \frac{1}{G_x} \arccos(\eta_x) ; \quad \sin(G_x q_{xc}) = \pm \sqrt{1 - \eta_x^2} , \\ q_{yc} &= \frac{1}{G_y} \arccos(\eta_y) ; \quad \sin(G_y q_{yc}) = \pm \sqrt{1 - \eta_y^2} , \end{aligned} \quad (36)$$

where

$$\eta_x = \frac{k_x}{2V_1(q_{zc}) G_x^2} , \quad \eta_y = \frac{k_y}{2V_1(q_{zc}) G_y^2} . \quad (37)$$

As we can see, equations (36) and (37) define a transition from a stable to instable tip's position, or in other words a transition from the stick to the slip state. Using this information we are able to explicitly calculate the parameters defining the friction force of the analytical model presented above. With this in mind, we explicitly define and calculate the parameter C_1 , C_2 , C_3 , C_{13} , C_{23} , E_1 , E_2 and E_3 which led to equation (7). From equation (31) we obtain,

$$\begin{aligned} C_1 &= \left. \frac{\partial^2 V_{Tot}}{\partial q_x \partial x} \right|_{\vec{q}_c, \vec{r}_c} = -k_x \\ C_2 &= \left. \frac{\partial^2 V_{Tot}}{\partial q_x \partial y} \right|_{\vec{q}_c, \vec{r}_c} = -k_y \\ C_3 &= \left. \frac{\partial^2 V_{Tot}}{\partial q_x \partial z} \right|_{\vec{q}_c, \vec{r}_c} = -k_z . \end{aligned}$$

Using equations (32), (33), (34), (36) and (37) we get

$$F_{xc} = C_1 x_c = -\frac{k_x}{G_x} \left(\arccos(\eta_x) + \frac{1}{\eta_x} \sqrt{1 - \eta_x^2} \right) \quad (38)$$

$$F_{yc} = C_2 y_c = -\frac{k_y}{G_y} \left(\arccos(\eta_y) + \frac{1}{\eta_y} \sqrt{1 - \eta_y^2} \right) \quad (39)$$

$$F_{lc} = \sqrt{F_{xc}^2 + F_{yc}^2} \quad (40)$$

$$F_{zc} = C_3 z_c = -k_z q_{zc} - V_0' - \frac{V_1'}{V_1} \left[\frac{k_x}{G_x^2} + \frac{k_y}{G_y^2} \right] \quad (41)$$

To calculate μ_0 and $\lambda_1(\theta)$ we start by calculating C_{13} , C_{23} and E_3 . From equations (31), (36) and (37) we can write

$$C_{13} = \left. \frac{\partial^2 V_{Tot}}{\partial q_x \partial q_z} \right|_{\vec{q}_c, \vec{r}_c} = -2U_1'(q_{zc}) G_x \sqrt{1 - \eta_x^2} \quad (42)$$

$$C_{23} = \left. \frac{\partial^2 V_{Tot}}{\partial q_y \partial q_z} \right|_{\vec{q}_c, \vec{r}_c} = -2U_1'(q_{zc}) G_y \sqrt{1 - \eta_y^2} \quad (43)$$

$$\begin{aligned} E_3 &= \left. \frac{\partial^2 V_{Tot}}{\partial q_z^2} \right|_{\vec{q}_c, \vec{r}_c} \\ &= k_z + V_0'' + \frac{V_1''}{V_1} \left[\frac{k_x}{G_x^2} + \frac{k_y}{G_y^2} \right] \neq 0 \end{aligned} \quad (44)$$

Using these results in equations (16) we obtain,

$$\mu_{0x} = \frac{-2V_1'(q_{zc}) G_x \sqrt{1 - \eta_x^2}}{|E_3|}, \quad (45)$$

$$\mu_{0y} = \frac{-2V_1'(q_{zc}) G_y \sqrt{1 - \eta_y^2}}{|E_3|}. \quad (46)$$

From equations (31), (36) and (37) we obtain E_1 and E_2 by,

$$E_1 = \left. \frac{\partial^3 V_{Tot}}{\partial q_x^3} \right|_{\vec{q}_c, \vec{r}_c} = \frac{k_x G_x}{\eta_x} \sqrt{1 - \eta_x^2} \quad (47)$$

$$E_2 = \left. \frac{\partial^3 V_{Tot}}{\partial q_y^3} \right|_{\vec{q}_c, \vec{r}_c} = \frac{k_y G_y}{\eta_y} \sqrt{1 - \eta_y^2} \quad (48)$$

where as defined by equation (17) we can calculate $\lambda_1(\theta)$ as,

$$\begin{aligned} \lambda_1(\theta) &= \frac{2^{\frac{7}{2}}}{3} \left\{ \left(\frac{\eta_x}{k_x G_x} \right)^{1/2} \frac{|\cos(\theta)|^{\frac{3}{2}}}{(1 - \eta_x^2)^{1/4}} + \right. \\ &\quad \left. \left(\frac{\eta_y}{k_y G_y} \right)^{1/2} \frac{|\sin(\theta)|^{\frac{3}{2}}}{(1 - \eta_y^2)^{1/4}} \right\}. \end{aligned} \quad (49)$$

Note that all the parameters F_{lc} , F_z^* , μ_0 , and λ_1 are functions of the critical point q_{zc} . Using the functions $V_0(q_z)$ and $V_1(q_z)$ of the Steele potential defined by [13],

$$V_0 = \frac{2\pi q \sigma_{ts}^6 \varepsilon_{ts}}{a_s} \sum_{p=0}^{\infty} \frac{1}{(q_z + p\Delta q_z)^4} \left(\frac{2\sigma_{ts}^6}{5(q_z + p\Delta q_z)^6} - 1 \right) \quad (50)$$

$$V'_0 = -\frac{8\pi q \sigma_{ts}^6 \varepsilon_{ts}}{a_s} \sum_{p=0}^{\infty} \frac{1}{(q_z + p\Delta q_z)^5} \left(\frac{\sigma_{ts}^6}{(q_z + p\Delta q_z)^6} - 1 \right) \quad (51)$$

$$V''_0 = \frac{8\pi q \sigma_{ts}^6 \varepsilon_{ts}}{a_s} \sum_{p=0}^{\infty} \frac{1}{(q_z + p\Delta q_z)^6} \left(\frac{11\sigma_{ts}^6}{(q_z + p\Delta q_z)^6} - 5 \right) \quad (52)$$

where p is an integer, q is the total number of atoms per unit surface cell, Δq_z is the distance between planes, $a_s = a_1^2$, is the area of the unit lattice cell, $a_1 = \sigma_{ss}$, σ_{ss} is the nearest neighbor in the solid and σ_{ts} and ε_{ts} are the parameters of a (6-12) Lennard-Jones potential between the tip and the surface atoms, and

$$V_1(q_z) = \frac{2\pi\sigma_{ts}^6\varepsilon_{ts}}{a_s} \left[\frac{\sigma_{ts}^6}{30} \left(\frac{g_1}{2q_z} \right)^5 K_5(g_1q_z) - 2 \left(\frac{g_1}{2q_z} \right)^2 K_2(g_1q_z) \right] \quad (53)$$

$$V'_1(q_z) = \frac{-2\pi\sigma_{ts}^6\varepsilon_{ts}}{a_s} \left\{ \frac{\sigma_{ts}^6}{30} \left(\frac{g_1}{2q_z} \right)^5 \times \left[\frac{10K_5(g_1q_z)}{q_z} + g_1K_4(g_1q_z) \right] - 2 \left(\frac{g_1}{2q_z} \right)^2 \left[\frac{4K_2(g_1q_z)}{q_z} + g_1K_1(g_1q_z) \right] \right\} \quad (54)$$

$$V''_1(q_z) = \frac{2\pi\sigma_{ts}^6\varepsilon_{ts}}{a_s} \left\{ \frac{\sigma_{ts}^6}{30} \left(\frac{g_1}{2q_z} \right)^5 \left[\frac{110K_5(g_1q_z)}{q_z^2} + \frac{19g_1K_4(g_1q_z)}{q_z} + g_1^2K_3(g_1q_z) \right] - 2 \left(\frac{g_1}{2q_z} \right)^2 \left[\frac{20K_2(g_1q_z)}{q_z^2} + \frac{7g_1K_1(g_1q_z)}{q_z} + g_1^2K_0(g_1q_z) \right] \right\} \quad (55)$$

where K_n is the modified Bessel function of second kind and $g_1 = G_x = G_y = 2\pi/a_1$. Using the equations from (50) to (55) we plot in figure 3 the parameters $\mu_{0x} = \mu_0$, and λ_1 and $V_{int}(\vec{q}_{||} = (a_1, a_1), q_z)$ as a function of q_z , for values of $\eta_x = \eta_y < 1$ since we are interested in real values of the parameters.

A. Theoretical prediction of the friction force and coefficient of friction

In the figure 3 we show the parameters μ_{0x} , λ_1 and V_{int} calculated by using the equations (45), (49) and (30) respectively. Using those results we can calculate the friction force, (f_L), and the coefficient of friction, (μ). The figure 4 shows (f_L) and (μ) as a function of the relative velocity v_L for several values of the of the normal force, (f_z). We note that these results agree quite well with the experimental data of *Riedo et.al* [4].

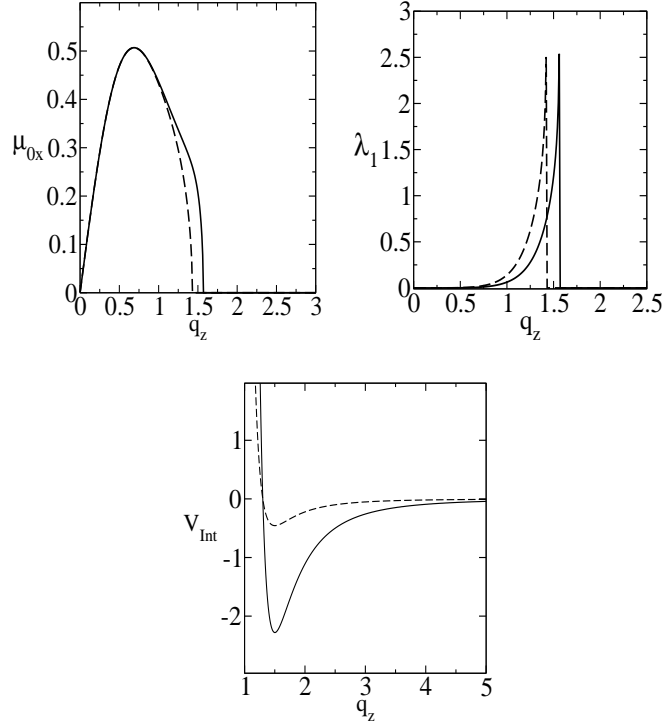


Figure 3: The parameters $\mu_{0x} = \mu_0$, λ_1 and $V_{int}(\vec{q}_{\parallel} = (a_1, a_1), q_z)$ plotted as a function of q_z . Here $\theta = 0$, $\sigma_{ts} = 1.2\sigma_{ss}$, $\varepsilon_{ts} = 0.5\varepsilon_{ss}$ (full), $0.1\varepsilon_{ss}$ (dashed).

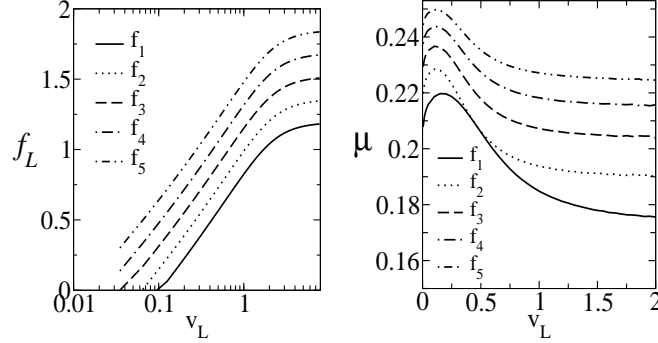


Figure 4: Theoretical friction force as a function of the velocity for different values of the normal force given by the equation (25). Here from bottom to top are shown $f_{N1} < f_{N2} < f_{N3} < f_{N4} < f_{N5}$ respectively.

In the figure 5 we present the dependence of the friction force (left) and the coefficient of friction (right) with the normal force (f_z). We note that the dependence of the coefficient of friction (right) with the normal force (f_z) agree quite well with the experimental data of *Eui-Sung Yoon et.al* [7].

In the figure 6 we present the dependence of the friction force (left) and the coefficient of friction (right) with the pushing angle, θ , relative to the direction (100) of the lattice. It is important to note that this result is a particular case for the potential defined by the equation (31). It is expected that the effect strongly depends on the symmetries of the surface.

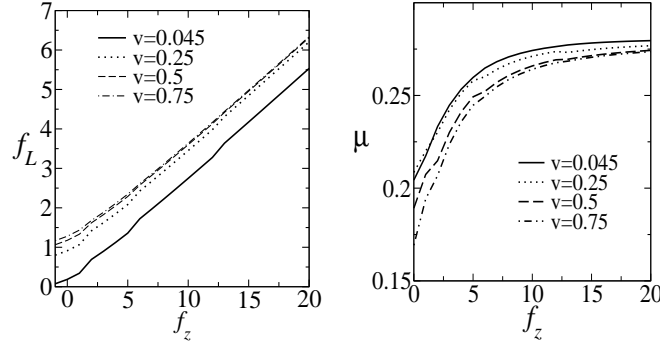


Figure 5: Friction force(left) and friction coefficient(right) as a function of the normal force for different values of the velocity. Here from bottom to top are shown $v_L = 0.045$, $v_L = 0.25$, $v_L = 0.5$, $v_L = 0.75$.

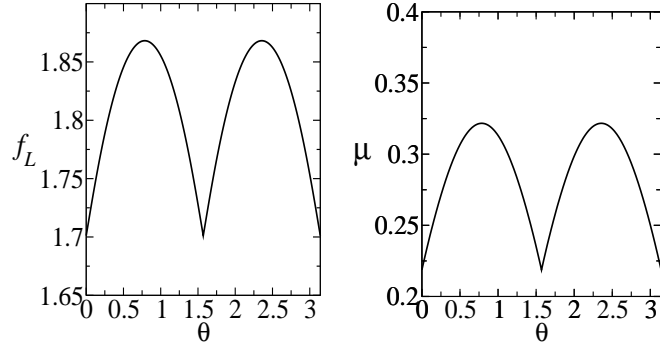


Figure 6: Dependence of the friction force(left) and the friction coefficient(right) on the direction of the sweepings, θ , relative to the (100) direction on the surface.

IV. SIMULATION

In this section we present our simulation for the system discussed above. The simulation is carried out using molecular dynamics (MD). The simulational arrangement is as shown in figure 1, which represents a tip interacting with a surface. The tip is simulated by a single particle. Three springs are attached to the particle, two parallels to the surface plan (x, y directions) and the other perpendicular to the surface plan (z direction). This arrangement allow us to measure the forces, normal (f_z) and parallel to the surface (f_x, f_y). The surface is represented by an arrangement of particles which interact with each other through a Lennard-Jones (LJ) (6 – 12) potential

$$\Phi_{i,j}(r_{i,j}) = \begin{cases} \phi_{i,j}(r_{i,j}) - \phi_{i,j}(r_c) - (r_{i,j} - r_c) \left(\frac{d\phi_{i,j}(r_{i,j})}{dr_{i,j}} \right)_{r_{i,j}=r_c} & \text{if } r_{i,j} < r_c \\ 0 & \text{if } r_{i,j} > r_c \end{cases} \quad (56)$$

$$\phi_{i,j}(r_{i,j}) = \epsilon_{i,j} \left[\left(\frac{\sigma_{i,j}}{r_{i,j}} \right)^{12} - \left(\frac{\sigma_{i,j}}{r_{i,j}} \right)^6 \right] \quad (57)$$

The indexes i and j stands for particles at position \vec{r}_i and \vec{r}_j respectively, and $1 \leq i, j \leq N$, where N is the total number of particles, $\sigma_{i,j} = \sigma_{ss}$, $\epsilon_{i,j} = \epsilon_{ss}$ between surface atoms and $\sigma_{i,j} = \sigma'_{ts}$, $\epsilon_{i,j} = \epsilon'_{ts}$ between the tip and surface atoms. A cutoff is introduced in the potential in order to accelerate the simulation. If the force on a particle is found by summing contributions from all particles acting upon it, then this truncation limits the computation time to an amount proportional to the total number of particles N . Of course, this truncation introduces discontinuities both in the potential and the force. To smooth these discontinuities we introduce the constant term $\phi(r_c)$. Another term $(d\phi_{i,j}(r_{i,j})/dr_{i,j})_{r_{i,j}=r_c}$ is introduced to remove the force discontinuity. Particles in the simulation move according

Newton's law of motion, which generates a set of $3N$ coupled equations of motion which are solved by increasing forward in time the physical state of the system in small time steps of size $\delta t = 10^{-3} \sigma_{ss} \sqrt{(m/\epsilon_{ss})}$. The resulting equations are solved by using Beeman's method of integration. In order to improve the simulations we use a Verlet table and cell division method. The temperature, T , of the surface can be controlled by using a velocity renormalization scheme [24, 25, 26, 27, 28, 29, 30, 31]. From the equipartition theorem we can write that

$$\langle v^2 \rangle = 3 \frac{k_B}{m} T. \quad (58)$$

We want to control the value of $\langle v^2 \rangle$ to correspond to a chosen temperature T_f . By initializing the system with $\langle v^2 \rangle_0$ we multiply each velocity by a factor α_0

$$\alpha_0 = \sqrt{\frac{m \langle v^2 \rangle_0}{3k_B T_f}}. \quad (59)$$

By evolving in time the system we can create a sequence $\{\alpha_n\}$, such that after a finite number of time steps the temperature of the system converges to T_f . We measure the time t , and temperature T , in units of $\sigma_{ss} \sqrt{m/\epsilon_{ss}}$ and ϵ_{ss}/k_B respectively.

A. Numerical background

Our simulation is as follows. We consider the system as consisting of an arrangement of particles of mass m , coupled by the Lennard-Jones potential defined by the equation (56). The system is arranged in 4 layers with free boundary conditions in all directions. The first layer is frozen in a regular arrangement as in the (001) surface of a Lennard-Jones bcc crystal in order to maintain the whole structure as flat as possible. The tip is simulated as a single particle of mass m , attached to three springs of elastic constant $k_x = \epsilon_{ss}/\sigma_{ss}^2$, $k_y = \epsilon_{ss}/\sigma_{ss}^2$ and $k_z = \epsilon_{ss}/\sigma_{ss}^2$ as shown schematically in figure 1. With the tip close to the surface we thermalize the system at temperature T . After thermalization the tip is pushed in a direction parallel to the surface at constant velocity $v_{0x} = v_L \cos(\theta)$, $v_{0y} = v_L \sin(\theta)$, $v_{0z} = 0$, $v_L = v \sqrt{(\epsilon_{ss}/m)}$. Here θ is defined relatively to the x direction and v is changed to obtain different velocities. For each simulation the distance between the tip and the surface is fixed at the beginning of the process, so that we can control the perpendicular force on the tip. By measuring the size variation of the springs we can calculate the laterals, f_x , f_y forces and the perpendicular, f_z force on the tip. This forces are measured in units of, $\epsilon_{ss}/\sigma_{ss}$. The velocity, position, energy and forces are stored at each time step for further analysis. Before we start the simulation we have to estimate the melting temperature T_m of the system. Figure 7 shows the total energy (per particle) as a function of temperature. The melting temperature is estimated as the inflexion point of the curve. We find $T_m \approx 1.1$ in accordance with earlier calculations [27, 28, 29]. Based in this result our simulations will be performed with $T < T_m$ and the temperature will be specified in each results. We have simulated the system for

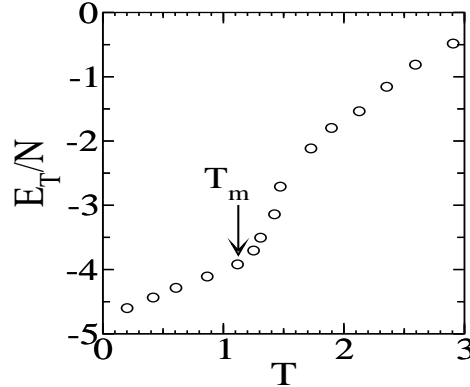


Figure 7: Energy as a function of temperature. The melting temperature is estimated as the inflexion point being around $T_m \approx 1.1$

several velocities, temperatures, initial distance of the tip to the substrate or equivalently, normal force in the tip and dragging angles relative to the surface. We are mainly interested in studding the effects of the velocity, the normal force and dragging angles relative to the surface in the friction force and coefficient of friction.

B. Dependence with velocity and normal force

In this section we show the results of our simulations for several values of the relative velocity tip-surface and for five different values of the normal force. In all the MD simulations of this subsection we use $\theta = 0$, $T = 0.5$. In the figure (8) we show the simulation (points) and the theoretical (full lines) results for the friction force as a function of the velocity for some normal forces. Note that our theoretical result, equation (25), is in very good agreement with the results of the MD simulations, only adjusting appropriate values for the critical position of jumps, q_{zc} (See section II). In the figure (9) we show the results of the simulation (points) and the theoretical results (full line) for

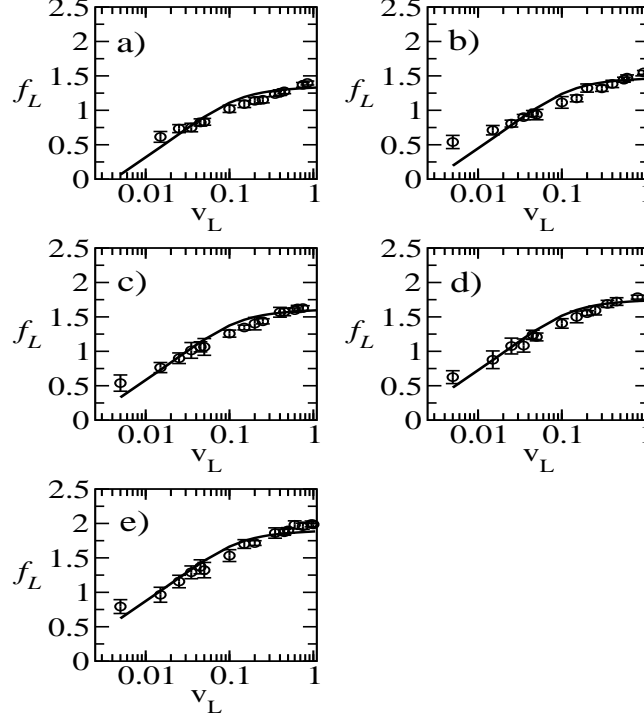


Figure 8: Friction force as a function of the velocity for some selected values of the normal force. From a) to e) we have respectively $\langle f_z \rangle \sim 0.95, 1.54, 2.25, 2.75$ and 2.50 . The points are the results of the simulations and the lines are from our analytical approach.

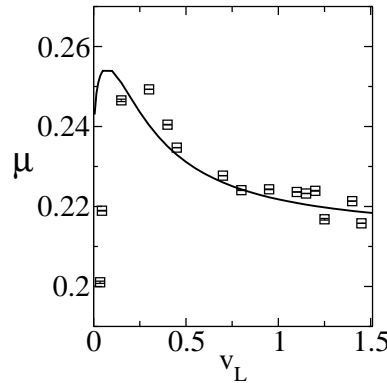


Figure 9: Averaged friction coefficient as a function of the velocity, calculated from the figure 8. The points are the results of the simulations and the line is the analytical result.

the averaged friction coefficient as function of the velocity. These results are in good agreement with the simulation, indicating that our model is consistent with the simulation.

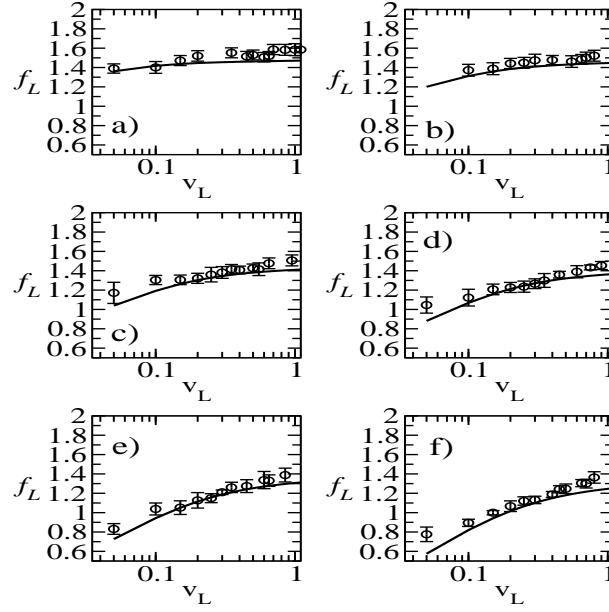


Figure 10: Friction force as a function of the velocity for some selected temperatures. The results of the simulations are shown as circles the lines are from our analytical approach. The results from a) to f) are respectively to $T = 0.1, 0.2, 0.3, 0.4, 0.5$ and 0.6 .

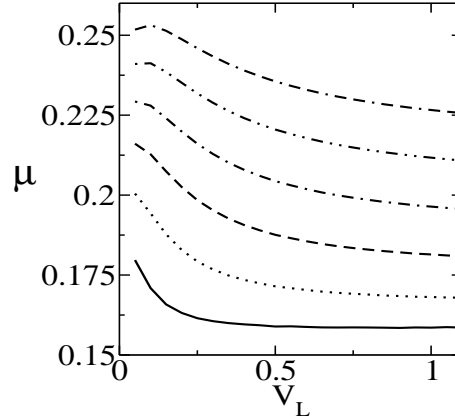


Figure 11: Averaged friction coefficient as a function of the velocity for some selected temperatures. Here, the lines are for the analytical results and from bottom to top corresponds respectively to $T = 0.1, T = 0.2, T = 0.3, T = 0.4, T = 0.5$ and $T = 0.6$.

C. Dependence with Temperature and Velocity.

In this section we present some simulation for the friction force for several velocities, and different values of temperature, ($T = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$). In all the simulations in this subsection we use $\theta = 0$ and $\langle f_z \rangle \sim 0.95$. In the figure (10) are the results of the MD simulations (points) and the theoretical result (full lines) for the friction force. Note that our theoretical results are in excellent agreement with the results of the MD simulation. In the figure (11) we show the analytical results for the averaged friction coefficient as a function of the velocity. In this figure, the lines from bottom to top corresponds respectively to $T = 0.1, T = 0.2, T = 0.3, T = 0.4, T = 0.5, T = 0.6$.

In figures (9) and (11), it is shown the behavior of the friction coefficient as a function of the relative velocity. We note that initially the friction coefficient increases with the velocity until it reaches a maximum and then starts to diminish. The initial increasing and the maximum value for the coefficient of friction can be related to the fact that when the velocity increases the tip executes jumps more and more energetic, and a high friction mode associated with single slips appears as indicated by Nakamura et. al. [32]. As the velocity pass through a certain limit a low friction mode with double slips appears leading to the observed reduction of the friction coefficient.

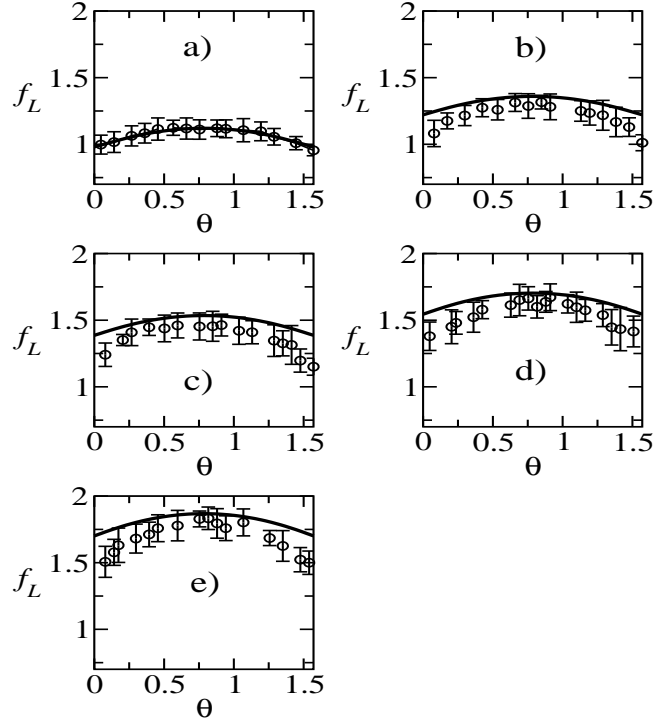


Figure 12: Friction force as function of the angle, θ , for some selected normal forces. From a) to e) we have respectively $\langle f_z \rangle \sim 0.95, 1.54, 2.25, 2.75, 2.50$. The points are the results of the simulations and the lines are our theoretical results.

D. Dependence with Normal Force and Force Pushing Angle.

Below we present the simulations for five different values of the normal force and several pulling angles, $0 \leq \theta \leq \pi/2$, between the direction x and the force pulling the cantilever. In all the MD simulations in this section we use $v_l = 0.05$, $T = 0.5$. In the figure (12) and (13) we show our results of the simulation (points) and the analytical calculations

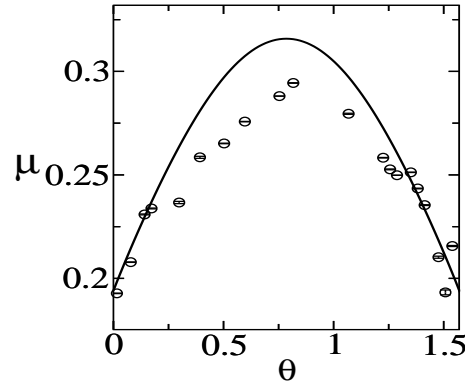


Figure 13: Averaged friction coefficient as a function of the angle, θ , calculated from the figure 12. The points are the results of the simulations and the line is the analytical result.

(full lines) for the friction force and the averaged friction coefficient as a function of the angle, θ . Note that our theoretical result, equation (25), is in very good agreement with the results of the MD simulations.

V. CONCLUSION AND COMMENTS

In this paper we have proposed a tri-dimensional model to describe friction force. Our approach generalize the one-dimensional friction force model proposed in earlier works [4, 8]. In our model we include the influence of the normal force which allow us to calculate the friction coefficient for first principles. We apply our model to calculate the friction force and friction coefficient for a tip-surface interaction. The interaction between the tip and the surface is represented by a Lennard-Jones potential and the surface represented by a potential that represent a (001) surface symmetry and the friction force obtained are in good agreement with the experimental results presentes by Riedo[4]. With the intend to test our model we performed classical molecular-dynamics simulation for a particle attached in a spring and pushed over a BCC(001) surface crystal. For this purpose we performed the simulation for several velocities, temperatures, normal forces and dragging angle. We have found that the friction forces and the friction coefficient are in good agreement with our molecular dynamic results, proving the effectiveness of our model.

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